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(54) Title: **METHOD, COMPUTING ROUTINE, DEVICE FOR PREDICTING PROPERTIES OF MHC/PEPTIDE COMPLEXES, AND DATA AND PEPTIDES PRODUCED THEREFROM**

(57) Abstract: The present invention relates to a method for structure-based prediction of properties of peptides and peptide analogs in complex with major histocompatibility (MHC) class I and class II molecules. The said properties mainly relate to the three-dimensional structure of an MHC/peptide complex and the binding affinity of a peptide for an MHC receptor. The invention further relates to a computer program and a device therefor. The invention further relates to data produced by a method of the invention. The invention further relates to peptides and peptide analogs predicted to bind to target-MHC molecules. The present invention thus relates to the field of immunology, with possible applications in manufacture of vaccines, de-immunization of proteins, and manufacture of therapeutic agents, especially immunotherapeutic agents.

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